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PROGRAM: INVITRO.CSL
!MODIFIED FROM PAUL INVITRO MODEL FOR MALE
!MODEL TO SIMULATE BETA CHLOROPRENE UPTAKE
!AND METABOLISM IN A ONE-COMPARTMENT
!REMOVE ALL THE PATHWAY RELATE TO CEO
!COSIDER SATURABLE PATHWAY FOR MICE LIVER/LUNG, RAT LIVER
!BUT ONLY V/K FOR RAT LUNG
!VIAL SYSTEM CONTAINING MICROSOMES ONLY
!VK RXN only happen in Rat Lung
!Including Background Rate : 0.001424477


VARIABLE TIME

INITIAL

CONSTANT VMAX1=0.          !MAX RATE OF MET. (uMOL/HR/mg protein)
CONSTANT KM1=0.1           !MICHAELIS CONSTANT (uMOL/L)
CONSTANT RLOSS = 0.001424   !Background loss rate (1/hr)
CONSTANT VK=0.              !REPRESENT THE V/K COEFFICIENT FOR RAT LUNG
(1/hr)

CONSTANT P1=0.69           !MEDIA/AIR PARTITION for CD

CONSTANT A10=0.            !INITIAL AMOUNT IN VIAL (uMOL)

CONSTANT VVIAL=0.01165     !VOLUME OF VIAL (L); Vial volume= 11.65 ml
CONSTANT VMED=0.001        !VOLUME OF MEDIA (L); Liquid voume
 VAIR=VVIAL-VMED               !HEADSPACE
CONSTANT PROT = 1.0        !AMOUNT OF PROTEIN (mg)

CONSTANT TF=0              !TIME OF FIRST SAMPLE (hr); kept same
CONSTANT TI=0.2            !INTERVAL BETWEEN SAMPLES (hr)kept same
CONSTANT VINJ=0.0002       !INJECTION VOLUME (L); based on Matt email

!Initial Conditions
 CA10=A10/(VAIR+P1*VMED)
 CM10=CA10*P1             !CONC in SOLUTION
 CA1=CA10
 CM1=CM10
 A1I=0.



!TIMING COMMANDS
CONSTANT TSTOP=1          !LENGTH OF EXPOSURE (HOURS)
CONSTANT POINTS=100.      !NO. OF POINTS IN PLOT
CINTERVAL CINT=0.01       !COMMUNICATION INTERVAL
TS=TF
SCHEDULE step .AT. TF

END                        !END INITIAL

DYNAMIC
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ALGORITHM IALG=2

  DERIVATIVE

  TERMT(TIME.GE.TSTOP)

!CD KINETICS (umoles/hr)
  R1M=(VMAX1*CM1)/(KM1+CM1)*PROT
  RRLUNGVK=VK*CM1
  RRLoss = RLOSS*CM1
  A1M=INTEG(R1M,0.)
  ARLUNGVK=INTEG(RRLUNGVK,0.)
  ARLOSS = INTEG(RRLoss,0.)

  CA1=(A10-A1M-ARLUNGVK-A1I-ARLOSS)/(VAIR+VMED*P1)
  CM1=CA1*P1
  A1=CA1*VAIR+CM1*VMED


!MASS BALANCE
  CHECK1 = A10 - (A1+A1M+A1I+ ARLUNGVK-ARLOSS)

DISCRETE step
PROCEDURAL
!Routine for sample loss
    A1I=A1I+CA1*VINJ
    SCHEDULE step .AT. TS+TI
    TS=TS+TI
END                        !END PROCEDURAL
END                        !END DISCRETE

END                        !END DERIVATIVE
END                        !END DYNAMIC
END                        !END PROGRAM
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